ChemSpider
The free chemical database

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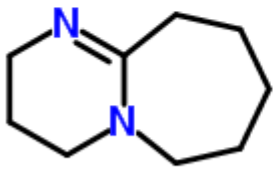
DBU



2D 3D Save Zoom

ChemSpider ID: **73246**

Molecular Formula: $C_9H_{16}N_2$

Average mass: 152.236694 Da

Monoisotopic mass: 152.131348 Da

▼ Systematic name

2,3,4,6,7,8,9,10-Octahydropyrimido[1,2-a]azepine

▶ SMILES and InChIs

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▼ Properties

Experimental data | **Predicted** - ACD/Labs | **Predicted** - EPISuite | **Predicted** - ChemAxon

Predicted data is generated using the ACD/Labs' ACD/PhysChem Suite, for more information see their website.

ACD/LogP:	1.132	# of Rule of 5 Violations:	0
ACD/LogD (pH 5.5):	-0.87	ACD/LogD (pH 7.4):	-0.87
ACD/BCF (pH 5.5):	1.00	ACD/BCF (pH 7.4):	1.00
ACD/KOC (pH 5.5):	1.00	ACD/KOC (pH 7.4):	1.00
#H bond acceptors:	2	#H bond donors:	0
#Freely Rotating Bonds:	0	Polar Surface Area:	15.6 Å^2
Index of Refraction:	1.592	Molar Refractivity:	45.932 cm^3
Molar Volume:	135.773 cm^3	Polarizability:	18.209 10^{-24}cm^3
Surface Tension:	42.2319984436035 dyne/cm	Density:	1.121 g/cm^3
Flash Point:	119.866 °C	Enthalpy of Vaporization:	51.299 kJ/mol
Boiling Point:	274.586 °C at 760 mmHg	Vapour Pressure:	0.00499999988824129 mmHg at 25°C